

# Ginzburg-Landau Equations for Coexistent States of Superconductivity and Antiferromagnetism in $t - J$ model

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Ginzburg-Landau (GL) equations for the coexistent state of superconductivity and antiferromagnetism are derived microscopically from the  $t - J$  model with extended transfer integrals. GL equations and the GL free energy, which are obtained based on the slave-boson mean-field approximation, reflect the electronic structure of the microscopic model, especially the evolution of the Fermi surface due to the change of the doping rate. Thus they are suitable for studying the material dependence of the coexistent states in high- $T_C$  cuprate superconductors.

KEYWORDS: GL theory,  $t$ - $J$  model, coexistence, antiferromagnetism

## 1. Introduction

The discovery of the coexistence of antiferromagnetism (AF) and superconductivity (SC) in multilayer high- $T_C$  cuprates has stimulated wide interest.<sup>1,2)</sup> Antiferromagnetic superexchange interactions in high- $T_C$  cuprate superconductors, which are strongly correlated electron systems, are thought to be the origin of two ordered states; thus understanding the condition for coexistence may give insight into the mechanism of superconductivity.

In single-layer and bilayer cuprates such as La- and Y-based compounds, it has been well known that AF is easily suppressed by a tiny amount of carrier doping.<sup>3,4)</sup> On the contrary in multilayer systems (in this paper the term "multilayer" will refer to three or more layers in a unit cell) such as  $\text{HgBa}_2\text{Ca}_4\text{Cu}_5\text{O}_{12+y}$ , AF survives up to much higher doping rate and coexists with SC state. NMR measurements revealed that the coexistence was not due to a proximity effect but a genuine phase transition within a  $\text{CuO}_2$  plane.<sup>1,2)</sup> Multilayer cuprates have flat  $\text{CuO}_2$  planes with a perfect square lattice and are known to be free from disorder in contrast to La- and Y-based compounds. Combined with their high  $T_C$  of more than 100K,<sup>5)</sup> multilayer cuprates can be viewed as ideal systems to study the mechanism of high  $T_C$ . In this sense it is desirable to explore the nature of the coexistent state of AF and SC theoretically.

Low-energy electronic states of high- $T_C$  cuprates are described by the  $t - J$  model.<sup>6-8)</sup>

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In the case of single-layer and bilayer systems the AF order is easily destabilized by strong fluctuations due to low dimensionality. Assuming the absence of AF order, mean-field (MF) theories<sup>9,10)</sup> based on the slave-boson (SB) scheme<sup>11)</sup> to treat the condition of no double occupancy and the gauge theory,<sup>8,12)</sup> which takes into account the low-energy fluctuations around mean-fields, capture many important properties of single-layer and bilayer high- $T_C$  cuprates. In multilayer systems, on the other hand, relatively strong three dimensionality may stabilize AF order.<sup>13,14)</sup> This situation can be suitably treated by MF theories for the  $t - J$  model by taking AF order into account. Actually MF calculations for the  $t - J$  model predicted that AF survives up to  $\delta \lesssim 0.1 - 0.15$  ( $\delta$  being the doping rate) and it may coexist with SC,<sup>13-16)</sup> and a similar result was obtained by the variational Monte Carlo method.<sup>17)</sup>

In this paper, we derive GL equations and the GL free energy microscopically from the two-dimensional  $t - J$  model with extended transfer integrals (extended  $t - J$  model) based on the SBMF approximation. In the MF approach the phase diagram will not be sensitive to the number of layers. It is the shape of the Fermi surface, in particular, the condition for the nesting that is crucial to determine the occurrence of the coexistent state, and an electronlike Fermi surface can lead to the experimentally observed phase diagram.<sup>13,14)</sup> In multilayer cuprates we expect that such an electronlike Fermi surface may be stabilized as one of the Fermi surface due to strong hybridization between layers. This is the reason why we treat a single-layer (single-band) model, and we simulate the difference of the Fermi surface by including the extended transfer integrals.

The derived GL theory can be used to investigate the spatial dependence of the AF and SC order parameters (OPs) in high- $T_C$  cuprates, and it may provide information on the electronic states in these systems. For example, near the surface or impurity the OPs are suppressed, and their recovery to the bulk values will provide the coherence length, which reflect the underlying electronic structures of each system.

Although the GL theory is reliable only qualitatively except near  $T_C$ , it can give a simple and intuitive description of the coexistence and competition of multiple OPs. Thus, it is complementary to more sophisticated methods such as the Bogoliubov-de Gennes and quasiclassical Green's function theory. Previously various models have been employed to derive GL equations microscopically; a continuum<sup>18)</sup> and tight-binding model<sup>19)</sup> with  $s$ - and  $d$ -wave SCOPs, Hubbard model with nearest-neighbor attractive interactions,<sup>20)</sup> a model with a spin generalized BCS term and Heisenberg exchange term,<sup>21)</sup> and the  $t - J$  model (without taking AF order into account).<sup>22)</sup> The method of deriving GL equations in this work is based on that by Gor'kov<sup>23)</sup> with the extension to include AF order.<sup>20)</sup>

This paper is organized as follows. In §2, we present the model and treat it by the SBMF approximation. GL equations and the GL free energy are derived in §3. Section 4 is devoted to summary and discussion.

## 2. Model and Mean-Field Approximation

We consider the extended  $t - J$  model on a square lattice whose Hamiltonian is given as

$$H = - \sum_{j,\ell,\sigma} t_{j\ell} e^{i\phi_{j\ell}} \tilde{c}_{j\sigma}^\dagger \tilde{c}_{\ell\sigma} + J \sum_{\langle j,\ell \rangle} \mathbf{S}_j \cdot \mathbf{S}_\ell, \quad (1)$$

where the transfer integrals  $t_{j\ell}$  are finite for the first- ( $t$ ), second- ( $t'$ ), and third-nearest-neighbor bonds ( $t''$ ), and vanish otherwise.  $J(> 0)$  is the antiferromagnetic superexchange interaction and  $\langle j, \ell \rangle$  denotes the nearest-neighbor bonds. The magnetic field is taken into account using the Peierls phase  $\phi_{j,\ell} \equiv \frac{\pi}{\phi_0} \int_j^\ell \mathbf{A} \cdot d\mathbf{l}$ , with  $\mathbf{A}$  and  $\phi_0 = \frac{hc}{2e}$  being the vector potential and flux quantum, respectively.  $\tilde{c}_{j\sigma}$  is the electron operator in Fock space without double occupancy, and we treat this condition using the SB method<sup>11)</sup> by writing  $\tilde{c}_{j\sigma} = b_j^\dagger f_{j\sigma}$  under the local constraint  $\sum_\sigma f_{j\sigma}^\dagger f_{j\sigma} + b_j^\dagger b_j = 1$  at every  $j$  site. Here  $f_{j\sigma}$  ( $b_j$ ) is a fermion (boson) operator that carries spin  $\sigma$  (charge  $e$ ); the fermions (bosons) are frequently referred to as spinons (holons). The spin operator is expressed as  $\mathbf{S}_j = \frac{1}{2} \sum_{\alpha,\beta} f_{j\alpha}^\dagger \sigma_{\alpha\beta} f_{j\beta}$ .

We decouple Hamiltonian eq. (1) in the following manner.<sup>13–16)</sup> The bond order parameters  $\langle \sum_\sigma f_{j\sigma}^\dagger f_{\ell\sigma} \rangle$  and  $\langle b_j^\dagger b_\ell \rangle$  are introduced and we denote  $\chi_{j,\ell}/2 = \langle f_{j\uparrow}^\dagger f_{\ell\uparrow} \rangle = \langle f_{j\downarrow}^\dagger f_{\ell\downarrow} \rangle$  for the nearest-neighbor bond. Although the bosons are not condensed in purely two-dimensional systems at finite temperature ( $T$ ), they are almost condensed at low  $T$  and for finite carrier doping  $\delta (\gtrsim 0.02)$ .<sup>15)</sup> Hence we approximate  $\langle b_j \rangle \approx \sqrt{\delta}$  and  $\langle b_i^\dagger b_j \rangle \approx \delta$ . The magnetization is defined by  $m_j = \frac{1}{2} \langle f_{j\uparrow}^\dagger f_{j\uparrow} - f_{j\downarrow}^\dagger f_{j\downarrow} \rangle$ , and the superconducting OP on the bond  $\langle j, \ell \rangle$  (under the assumption of the Bose condensation of holons) is given as  $\Delta_{j,\ell} = \langle f_{j\uparrow} f_{\ell,\downarrow} \rangle$ .

In the following we are mainly interested in a region around the tetracritical point where the four states, AF,  $d_{x^2-y^2}$ -wave SC, their coexistence, and the normal states become identical. The onset temperature of the bond OPs is much higher than that for AF ( $T_N$ ) and SC ( $T_C$ ) in this doping region, so that they are almost independent of temperature near the tetracritical point. We consider only the spatial variations of  $m_j$  and  $\Delta_{j,\ell}$  assuming that  $\chi_{j,\ell}$  is uniform in

space. (Hereafter we denote it as  $\chi$ .) Then the mean-field Hamiltonian is given as

$$\begin{aligned}
 H_{MFA} = & - \sum_{j,\sigma} \left[ \sum_{\delta=\pm x, \pm y} (t\delta e^{i\phi_{j+\delta,j}} + \frac{3J}{8}\chi) f_{j+\delta,\sigma}^\dagger f_{j\sigma} + t'\delta \sum_{\delta=\pm x, \pm y} e^{i\phi_{j+\delta,j}} f_{j+\delta,\sigma}^\dagger f_{j\sigma} \right. \\
 & + \left. t''\delta \sum_{\delta=\pm 2x, \pm 2y} e^{i\phi_{j+\delta,j}} f_{j+\delta,\sigma}^\dagger f_{j\sigma} \right] - \mu \sum_{j,\sigma} f_{j\sigma}^\dagger f_{j\sigma} + \frac{J}{2} \sum_j \sum_{\delta=\pm x, \pm y} m_{j+\delta} (f_{j\uparrow}^\dagger f_{l\uparrow} - f_{j\downarrow}^\dagger f_{l\downarrow}) \\
 & + \frac{J}{2} \sum_j \sum_{\delta=\pm x, \pm y} [\Delta_{j,j+\delta} (f_{j+\delta\uparrow}^\dagger f_{j\downarrow}^\dagger - \frac{1}{2} f_{j+\delta\downarrow}^\dagger f_{j\uparrow}^\dagger) + h.c.] + E_0,
 \end{aligned} \tag{2}$$

with

$$E_0 = -J \sum_{\langle j,\ell \rangle} m_j m_\ell + J \sum_{\langle j,\ell \rangle} \left( \frac{1}{2} \Delta_{j,\ell} \Delta_{\ell,j}^* + \frac{1}{4} |\Delta_{j,\ell}|^2 \right). \tag{3}$$

First we solve the self-consistency equations for  $\chi$  and the chemical potential  $\mu$  in the absence of  $m$ ,  $\Delta$ , and  $\mathbf{A}$ . Self-consistency equations that determine  $\chi$  and  $\mu$  as functions of  $T$  and  $\delta$  are given as

$$\chi = \frac{1}{N} \sum_p (\cos p_x + \cos p_y) f(\xi_p), \quad \delta = 1 - \frac{2}{N} \sum_p f(\xi_p), \tag{4}$$

where  $\xi_p = -(2t\delta + \frac{3J}{4}\chi)(\cos p_x + \cos p_y) - 4t'\delta \cos p_x \cos p_y - 2t''\delta(\cos 2p_x + \cos 2p_y) - \mu$ , with  $f$  and  $N$  being the Fermi function and the total number of lattice sites, respectively. (Lattice constant is taken to be unity.) In the next section we will carry out the GL expansion to obtain GL equations for  $m$  and  $\Delta$ .

### 3. GL Equations and GL Free Energy

In this section we derive GL equations and the GL free energy. The procedure is essentially the same as that used in ref.20. Coupled equations for Green's functions  $G_\sigma(j, \ell, \tau) = -\langle T_\tau f_{j\sigma}(\tau) f_{\ell\sigma}^\dagger \rangle$  and  $F_{\sigma\sigma'}^\dagger(j, \ell, \tau) = -\langle T_\tau f_{j\sigma}^\dagger(\tau) f_{\ell\sigma'}^\dagger \rangle$  can be derived from their equations of motion (Gor'kov equations) as

$$\begin{aligned}
G_{\uparrow}(j, \ell, i\varepsilon_n) &= \tilde{G}_0(j, \ell, i\varepsilon_n) + \frac{J}{2} \sum_{k, \delta_1} \tilde{G}_0(j, k, i\varepsilon_n) \\
&\quad \times \left[ \left( \Delta_{k+\delta_1, k} + \frac{1}{2} \Delta_{k, k+\delta_1} \right) F_{\downarrow\uparrow}^{\dagger}(k + \delta_1, \ell, i\varepsilon_n) + m_{k+\delta_1} G_{\uparrow}(k, \ell, i\varepsilon_n) \right], \\
G_{\downarrow}(j, \ell, i\varepsilon_n) &= \tilde{G}_0(j, \ell, i\varepsilon_n) - \frac{J}{2} \sum_{k, \delta_1} \tilde{G}_0(j, k, i\varepsilon_n) \\
&\quad \times \left[ \left( \Delta_{k, k+\delta_1} + \frac{1}{2} \Delta_{k+\delta_1, k} \right) F_{\uparrow\downarrow}^{\dagger}(k + \delta_1, \ell, i\varepsilon_n) + m_{k+\delta_1} G_{\downarrow}(k, \ell, i\varepsilon_n) \right], \\
F_{\downarrow\uparrow}^{\dagger}(j, \ell, i\varepsilon_n) &= -\frac{J}{2} \sum_{k, \delta_1} \tilde{G}_0(k, j, -i\varepsilon_n) \\
&\quad \times \left[ \left( \Delta_{k, k+\delta_1}^* + \frac{1}{2} \Delta_{k+\delta_1, k}^* \right) G_{\uparrow}(k + \delta_1, \ell, i\varepsilon_n) + m_{k+\delta_1} F_{\downarrow\uparrow}^{\dagger}(k, \ell, i\varepsilon_n) \right], \\
F_{\uparrow\downarrow}^{\dagger}(j, \ell, i\varepsilon_n) &= \frac{J}{2} \sum_{k, \delta_1} \tilde{G}_0(k, j, -i\varepsilon_n) \\
&\quad \times \left[ \left( \Delta_{k+\delta_1, k}^* + \frac{1}{2} \Delta_{k, k+\delta_1}^* \right) G_{\downarrow}(k + \delta_1, \ell, i\varepsilon_n) + m_{k+\delta_1} F_{\uparrow\downarrow}^{\dagger}(k, \ell, i\varepsilon_n) \right],
\end{aligned} \tag{5}$$

where the summation on  $\delta_1$  ( $k$ ) is over  $\pm\hat{x}$  and  $\pm\hat{y}$  (all sites). Here,  $\tilde{G}_0(j, \ell, i\omega_n)$  is Green's function for the system without  $\Delta$  and  $m$  but with  $\mathbf{A}$ .  $\tilde{G}_0(j, \ell, i\omega_n)$  is related to Green's function for the system without  $\mathbf{A}$ ,  $G_0$ , as  $\tilde{G}_0(j, \ell, i\varepsilon_n) \sim G_0(j, \ell, i\varepsilon_n) e^{i\phi_{j,\ell}}$ , with  $G_0(j, \ell, i\varepsilon_n)$  being the Fourier transform of  $G_0(\mathbf{p}, i\varepsilon_n) = 1/(i\varepsilon_n - \xi_p)$ . In the expression of  $\xi_p$ , the bond order parameter  $\chi$  and the chemical potential  $\mu$  determined by eq.(4) are substituted.

Spin-singlet and spin-triplet SCOPs on the bond  $(j, j+\eta)$  are expressed in terms of Green's functions  $F_{\uparrow\downarrow}^{\dagger}$  and  $F_{\downarrow\uparrow}^{\dagger}$ ,

$$\begin{aligned}
(\Delta_{\eta}^{(S)}(j))^* &\equiv \frac{1}{2} \langle f_{j\uparrow} f_{j+\eta\downarrow} - f_{j\downarrow} f_{j+\eta\uparrow} \rangle^* = \frac{1}{2} (\Delta_{j,j+\eta} + \Delta_{j+\eta,j})^* \\
&= \frac{T}{2} \sum_{\varepsilon_n} [F_{\uparrow\downarrow}^{\dagger}(j + \eta, j, i\varepsilon_n) - F_{\downarrow\uparrow}^{\dagger}(j + \eta, j, i\varepsilon_n)], \\
(\Delta_{\eta}^{(T)}(j))^* &\equiv \frac{1}{2} \langle f_{j\uparrow} f_{j+\eta\downarrow} + f_{j\downarrow} f_{j+\eta\uparrow} \rangle^* = \frac{1}{2} (\Delta_{j,j+\eta} - \Delta_{j+\eta,j})^* \\
&= -\frac{T}{2} \sum_{\varepsilon_n} [F_{\uparrow\downarrow}^{\dagger}(j + \eta, j, i\varepsilon_n) + F_{\downarrow\uparrow}^{\dagger}(j + \eta, j, i\varepsilon_n)],
\end{aligned} \tag{6}$$

and the staggered magnetization  $M_j \equiv m_j e^{i\mathbf{Q} \cdot \mathbf{r}_j}$  ( $\mathbf{Q} = (\pi, \pi)$ ) is similarly given using  $G_{\uparrow}$  and  $G_{\downarrow}$ ,

$$\begin{aligned}
M_j &\equiv \frac{1}{2} \langle f_{j\uparrow}^{\dagger} f_{j\uparrow} - f_{j\downarrow}^{\dagger} f_{j\downarrow} \rangle e^{i\vec{Q} \cdot \vec{r}_j} \\
&= \frac{T}{2} \sum_{\varepsilon_n} [G_{\uparrow}(j, j, i\varepsilon_n) - G_{\downarrow}(j, j, i\varepsilon_n)] e^{i\vec{Q} \cdot \vec{r}_j}.
\end{aligned} \tag{7}$$

We substitute eq. (5) into eqs. (6) and (7) iteratively and keep the terms up to the third order in OPs. In the coexistent state of AF and SC, spin-triplet SCOPs that oscillate in a similar manner as the staggered magnetization may occur,<sup>24–28)</sup> and they are called the  $\pi$ -triplet SCOPs.

The SCOPs of each symmetry,  $\Delta_s$  (*s*-wave),  $\Delta_d$  (*d*-wave), and  $\Delta_{px(y)}^{(\pi T)}$  ( $\pi$ -triplet *px*(*y*)-wave), can be constructed by making a linear combination of eq.(6),

$$\begin{aligned}\Delta_s(j) &= \frac{1}{4} \sum_{\eta=\pm\hat{x},\pm\hat{y}} \Delta_\eta^{(S)}(j), \quad \Delta_d(j) = \frac{1}{4} \left[ \sum_{\eta=\pm\hat{x}} \Delta_\eta^{(S)}(j) - \sum_{\eta=\pm\hat{y}} \Delta_\eta^{(S)}(j) \right], \\ \Delta_{px(y)}^{(\pi T)}(j) &= \frac{1}{2} [\Delta_{\hat{x}(y)}^{(\pi T)}(j) + \Delta_{-\hat{x}(y)}^{(\pi T)}(j)].\end{aligned}\quad (8)$$

Assuming that the SCOPs and  $M$  are slowly varying, we take a continuum limit. The OPs in the linear terms are expanded in powers of derivatives up to the second order, and the Peierls phase is also expanded in powers of  $\mathbf{A}$  to the same order. Then after straightforward but lengthy calculations we get the following GL equations:

$$\begin{aligned}& \alpha_s \Delta_s + 2\beta_s |\Delta_s|^2 \Delta_s - K_s (D_x^2 + D_y^2) \Delta_s - K_{ds} (D_x^2 - D_y^2) \Delta_d \\ & + \gamma_1 |\Delta_d|^2 \Delta_s + 2\gamma_2 \Delta_d^2 \Delta_s^* + \gamma_3 (|\Delta_{px}|^2 + |\Delta_{py}|^2) \Delta_s + 2\gamma_5 (\Delta_{px}^2 + \Delta_{py}^2) \Delta_s^* \\ & + \gamma_7 (|\Delta_{px}|^2 - |\Delta_{py}|^2) \Delta_d + \gamma_8 (\Delta_{px}^2 - \Delta_{py}^2) \Delta_d^* + \gamma_9 (\Delta_{px}^* \Delta_{py} + c.c.) \Delta_s \\ & + 2\gamma_{11} \Delta_{px} \Delta_{py} \Delta_s^* + \gamma_{ms} M^2 \Delta_s + \gamma_{spm} M (\Delta_{px} + \Delta_{py}) = 0,\end{aligned}\quad (9)$$

$$\begin{aligned}& \alpha_d \Delta_d + 2\beta_d |\Delta_d|^2 \Delta_d - K_d (D_x^2 + D_y^2) \Delta_d - K_{ds} (D_x^2 - D_y^2) \Delta_s \\ & + \gamma_1 |\Delta_s|^2 \Delta_d + 2\gamma_2 \Delta_s^2 \Delta_d^* + \gamma_4 (|\Delta_{px}|^2 + |\Delta_{py}|^2) \Delta_d + 2\gamma_6 (\Delta_{px}^2 + \Delta_{py}^2) \Delta_d^* \\ & + \gamma_7 (|\Delta_{px}|^2 - |\Delta_{py}|^2) \Delta_s + \gamma_8 (\Delta_{px}^2 - \Delta_{py}^2) \Delta_s^* + \gamma_{10} (\Delta_{px}^* \Delta_{py} + c.c.) \Delta_d \\ & + 2\gamma_{12} \Delta_{px} \Delta_{py} \Delta_d^* + \gamma_{md} M^2 \Delta_d + \gamma_{dpm} M (\Delta_{px} - \Delta_{py}) = 0,\end{aligned}\quad (10)$$

$$\begin{aligned}& \alpha_{p1} \Delta_{px(y)} + \alpha_{p2} \Delta_{py(x)} + 2\beta_p |\Delta_{px(y)}|^2 \Delta_{px(y)} \\ & - K_{p1} D_{x(y)}^2 \Delta_{px(y)} - K_{p2} D_{y(x)}^2 \Delta_{px(y)} - K_{p3} (D_x^2 + D_y^2) \Delta_{py(x)} \\ & + \gamma_{p1} |\Delta_{py(x)}|^2 \Delta_{px(y)} + 2\gamma_{p2} \Delta_{py(x)}^2 \Delta_{px(y)}^* \\ & + \gamma_{p3} (2|\Delta_{px(y)}|^2 \Delta_{py(x)} + \Delta_{px(y)}^2 \Delta_{py(x)}^* + |\Delta_{py(x)}|^2 \Delta_{py(x)}) \\ & + (\gamma_3 |\Delta_s|^2 + \gamma_4 |\Delta_d|^2) \Delta_{px(y)} + 2(\gamma_5 \Delta_s^2 + \gamma_6 \Delta_d^2) \Delta_{px(y)}^* \\ & \pm \gamma_7 (\Delta_s \Delta_d^* + c.c.) \Delta_{px(y)} \pm 2\gamma_8 \Delta_s \Delta_d \Delta_{px(y)}^* + (\gamma_9 |\Delta_s|^2 + \gamma_{10} |\Delta_d|^2) \Delta_{py(x)} \\ & + (\gamma_{11} \Delta_s^2 + \gamma_{12} \Delta_d^2) \Delta_{py(x)}^* + (\gamma_{mp1} \Delta_{px(y)} + \gamma_{mp2} \Delta_{py(x)}) M^2 \\ & + (\gamma_{spm} \Delta_s \pm \gamma_{dpm} \Delta_d) M = 0,\end{aligned}\quad (11)$$

$$\begin{aligned}& \alpha_m M + 2\beta_m M^3 - K_m (\nabla_x^2 + \nabla_y^2) M \\ & + (\gamma_{ms} |\Delta_s|^2 + \gamma_{md} |\Delta_d|^2) M + [\gamma_{mp1} (|\Delta_{px}|^2 + |\Delta_{py}|^2) + \gamma_{mp2} (\Delta_{px} \Delta_{py}^* + c.c.)] M \\ & + \frac{1}{2} \gamma_{spm} [\Delta_s^* (\Delta_{px} + \Delta_{py}) + c.c.] + \frac{1}{2} \gamma_{dpm} [\Delta_d^* (\Delta_{px} - \Delta_{py}) + c.c.] = 0,\end{aligned}\quad (12)$$

where the coefficients appearing in eqs. (9)-(12) are given in the Appendix, and  $\mathbf{D}$  is the gauge-invariant gradient defined as  $\mathbf{D} \equiv \nabla + \frac{2\pi i}{\phi_0} \mathbf{A}$ . Equations (9)-(12) are the coupled equations

tions that determine SCOPs and the staggered magnetization self-consistently.

The GL free energy  $F$  up to the fourth order in OPs can be obtained from the above GL equations in such a way that the variations of  $F$  with respect to OPs reproduce eqs. (9)-(12).

The results are written as follows:

$$\begin{aligned}
F &= F_S + F_T + F_{ST} + F_M + F_{SM} + F_{TM} + F_{STM}, \\
F_S &= \int d^2\mathbf{r} \left[ \alpha_s |\Delta_s|^2 + \beta_s |\Delta_s|^4 + K_s |\vec{D}\Delta_s|^2 + \alpha_d |\Delta_d|^2 + \beta_d |\Delta_d|^4 + K_d |\vec{D}\Delta_d|^2 \right. \\
&\quad \left. + \gamma_1 |\Delta_s|^2 |\Delta_d|^2 + \gamma_2 (\Delta_d^* \Delta_s)^2 + c.c. \right) \\
&\quad \left. + K_{ds} ((D_x \Delta_d)(D_x \Delta_s)^* - (D_y \Delta_d)(D_y \Delta_s)^* + c.c.) \right], \\
F_T &= \int d^2\mathbf{r} \left[ \alpha_{p1} (|\Delta_{px}^{(\pi T)}|^2 + |\Delta_{py}^{(\pi T)}|^2) + \alpha_{p2} (\Delta_{px}^{(\pi T)} (\Delta_{py}^{(\pi T)})^* + c.c.) + \beta_p (|\Delta_{px}|^4 + |\Delta_{py}|^4) \right. \\
&\quad \left. + \gamma_{p1} |\Delta_{px}^{(\pi T)}|^2 |\Delta_{py}^{(\pi T)}|^2 + \gamma_{p2} ((\Delta_{px}^{(\pi T)})^2 (\Delta_{py}^{(\pi T)})^*)^2 + c.c. \right) \\
&\quad \left. + \gamma_{p3} (|\Delta_{px}^{(\pi T)}|^2 + |\Delta_{py}^{(\pi T)}|^2) (\Delta_{px}^{(\pi T)} (\Delta_{py}^{(\pi T)})^* + c.c.) \right. \\
&\quad \left. + K_{p1} (|D_x \Delta_{px}^{(\pi T)}|^2 + |D_y \Delta_{py}^{(\pi T)}|^2) + K_{p2} (|D_y \Delta_{px}^{(\pi T)}|^2 + |D_x \Delta_{py}^{(\pi T)}|^2) \right. \\
&\quad \left. + K_{p3} ((D_x \Delta_{px}^{(\pi T)})^* (D_x \Delta_{py}^{(\pi T)}) + (D_y \Delta_{px}^{(\pi T)})^* (D_y \Delta_{py}^{(\pi T)}) + c.c.) \right], \\
F_{ST} &= \int d^2\mathbf{r} \left[ (|\Delta_{px}^{(\pi T)}|^2 + |\Delta_{py}^{(\pi T)}|^2) (\gamma_3 |\Delta_s|^2 + \gamma_4 |\Delta_d|^2) \right. \\
&\quad \left. + \{ ((\Delta_{px}^{(\pi T)})^2 + (\Delta_{py}^{(\pi T)})^2) (\gamma_5 (\Delta_s^*)^2 + \gamma_6 (\Delta_d^*)^2) + c.c. \} \right. \\
&\quad \left. + \gamma_7 (|\Delta_{px}^{(\pi T)}|^2 - |\Delta_{py}^{(\pi T)}|^2) (\Delta_s^* \Delta_d + c.c.) + \gamma_8 \{ ((\Delta_{px}^{(\pi T)})^2 - (\Delta_{py}^{(\pi T)})^2) \Delta_s^* \Delta_d + c.c. \} \right. \\
&\quad \left. + ((\Delta_{px}^{(\pi T)})^* \Delta_{py}^{(\pi T)} + c.c.) (\gamma_9 |\Delta_s|^2 + \gamma_{10} |\Delta_d|^2) \right. \\
&\quad \left. + \{ \Delta_{px}^{(\pi T)} \Delta_{py}^{(\pi T)} (\gamma_{11} (\Delta_s^*)^2 + \gamma_{12} (\Delta_d^*)^2) + c.c. \} \right], \\
F_M &= \int d^2\mathbf{r} \left[ \alpha_m M^2 + \beta_m M^4 + K_m (\nabla M)^2 \right], \\
F_{SM} &= \int d^2\mathbf{r} \left( \gamma_{ms} M^2 |\Delta_s|^2 + \gamma_{md} M^2 |\Delta_d|^2 \right), \\
F_{TM} &= \int d^2\mathbf{r} \left[ \gamma_{mp1} M^2 (|\Delta_{px}^{(\pi T)}|^2 + |\Delta_{py}^{(\pi T)}|^2) \right. \\
&\quad \left. + \gamma_{mp2} M^2 (\Delta_{px}^{(\pi T)} (\Delta_{py}^{(\pi T)})^* + c.c.) \right], \\
F_{STM} &= \int d^2\mathbf{r} \left[ \gamma_{spm} M \Delta_s (\Delta_{px}^{(\pi T)} + \Delta_{py}^{(\pi T)})^* \right. \\
&\quad \left. + \gamma_{dpm} M \Delta_d (\Delta_{px}^{(\pi T)} - \Delta_{py}^{(\pi T)})^* + c.c. \right].
\end{aligned} \tag{13}$$

Here,  $F_S$ ,  $F_T$ , and  $F_M$  are the free energy for the singlet and  $\pi$ -triplet SCOPs, and the staggered magnetization, respectively, while  $F_{ST}$ ,  $F_{SM}$ ,  $F_{TM}$ , and  $F_{STM}$  describe their couplings. Note that  $F$  is invariant under all the symmetry operations of the square lattice.  $F_{SM}$  and  $F_{TM}$  are the usual terms to represent the competition of SCOPs and  $M$ .  $F_{STM}$  is a cubic term that couples spin-singlet SCOPs, staggered magnetization, and  $\pi$ -triplet SCOPs, and it induces  $\pi$ -triplet SCOPs in the coexistent state of AF and SC. Generally in the coexistent state of

ferromagnetism and spin-singlet SC state, spin-triplet SCOPs may occur when OPs are not uniform in space.<sup>29–33)</sup> In the GL theory this can be explained by a cubic term that has a gradient coupling of spin-singlet, triplet SCOPs, and the magnetization  $m$ .<sup>20)</sup> In the AF state magnetization  $m$  is oscillating (though the staggered magnetization  $M$  is uniform) even in a uniform case, and thus  $\pi$ -triplet SCOP can arise irrespective of the spatial dependence of OPs.

The important point of the present results is that the coefficients appearing in GL equations and the GL free energy are determined microscopically. These values depend on the parameters of the microscopic model and they reflect the evolution of the shape of the Fermi surface. This property can be used to study the material dependence of the coexistent states in various multilayer high- $T_C$  cuprates.

#### 4. Summary and Discussion

We have derived GL equations and the GL free energy microscopically from the extended  $t - J$  model using the slave-boson mean-field approximation. The derived GL theory can be used to investigate the spatial dependence of the AF and SC order parameters in high- $T_C$  cuprate superconductors. By analyzing the spatial variations of order parameters using the present results, information on the electronic states of high- $T_C$  cuprates may be extracted.

A typical example to be studied is the state near the surface or impurity. The interface states of heterostructures composed of cuprate superconductors and magnetic materials are also worth studying. There the coexistence and competition of superconductivity and magnetism can occur in various ways depending on the materials used.

Numerical study of the GL equations for the above situations assuming various band structure (by choosing the extended transfer integrals) may be interesting, and this problem will be examined separately.

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### Appendix: Coefficients in GL Equations and GL Free Energy

The coefficients appearing in GL equations [eqs.(9)-(12)] and the GL free energy [eq.(13)] are given as follows:

$$\begin{aligned}
 \alpha_{s(d)} &= 3J \left( 1 - \frac{3J}{4N} \sum_p I_1(p) \omega_{s(d)}^2 \right), \\
 \beta_{s(d)} &= \frac{81J^4}{32N} \sum_p I_2(p) \omega_{s(d)}^4, \\
 \gamma_1 &= \frac{81J^4}{8N} \sum_p I_2(p) \omega_s^2 \omega_d^2, \quad \gamma_2 = \frac{1}{4} \gamma_1, \\
 K_{s(d)} &= \frac{9J^2}{8N} \sum_p I_2(p) \left( \frac{\partial \xi_p}{\partial p_x} \right)^2 \omega_{s(d)}^2, \\
 K_{ds} &= \frac{9J^2}{8N} \sum_p I_2(p) \left( \frac{\partial \xi_p}{\partial p_x} \right)^2 \omega_s \omega_d, \\
 \alpha_{p1} &= -\frac{J}{2} \left( 1 + \frac{J}{2N} \sum_p I_3(p) \cos^2 p_x \right), \\
 \alpha_{p2} &= -\frac{J^2}{4N} \sum_p I_3(p) \cos p_x \cos p_y, \\
 \beta_p &= \frac{J^4}{32N} \sum_p I_4(p) \cos^4 p_x, \\
 \gamma_{p1} &= \frac{J^4}{8N} \sum_p I_4(p) \cos^2 p_x \cos^2 p_y, \quad \gamma_{p2} = \frac{1}{4} \gamma_{p1}, \\
 \gamma_{p3} &= \frac{J^4}{16N} \sum_p I_4(p) \cos^3 p_x \cos p_y, \\
 K_{p1(2)} &= -\frac{J^2}{8N} \sum_p I_4(p) \left( \frac{\partial \xi_p}{\partial p_x} \right)^2 \cos^2 p_{x(y)}, \\
 K_{p3} &= -\frac{J^2}{8N} \sum_p I_4(p) \left( \frac{\partial \xi_p}{\partial p_x} \right)^2 \cos p_x \cos p_y, \\
 \gamma_{3(4)} &= \frac{9J^4}{8N} \sum_p I_5(p) \omega_{s(d)}^2 \cos^2 p_x, \\
 \gamma_{5(6)} &= \frac{9J^4}{32N} \sum_p I_6(p) \omega_{s(d)}^2 \cos^2 p_x, \\
 \gamma_7 &= \frac{9J^4}{8N} \sum_p I_5(p) \omega_s \omega_d \cos^2 p_x, \\
 \gamma_8 &= \frac{9J^4}{16N} \sum_p I_6(p) \omega_s \omega_d \cos^2 p_x, \\
 \gamma_{9(10)} &= \frac{9J^4}{8N} \sum_p I_5(p) \omega_{s(d)}^2 \cos p_x \cos p_y, \\
 \gamma_{11(12)} &= \frac{9J^4}{16N} \sum_p I_6(p) \omega_{s(d)}^2 \cos p_x \cos p_y, \\
 \alpha_m &= 2J \left( 1 + \frac{2J}{N} \sum_p I_7(p) \right),
 \end{aligned} \tag{A.1}$$

$$\begin{aligned}
\beta_m &= \frac{8J^4}{N} \sum_p I_8(p), \\
K_m &= \frac{4J^2}{N} \sum_p I_8(p) \left( \frac{\partial \xi_p}{\partial p_x} \right)^2, \\
\{\gamma_{ms}, \gamma_{md}\} &= -\frac{9J^4}{N} \sum_p [2I_9(p) + I_6(p)] \{\omega_s^2, \omega_d^2\}, \\
\{\gamma_{mp1}, \gamma_{mp2}\} &= -\frac{J^4}{N} \sum_p [2I_{10}(p) + I_6(p)] \{\cos^2 p_x, \cos p_x \cos p_y\}, \\
\{\gamma_{spm}, \gamma_{dpm}\} &= -\frac{3J^3}{N} \sum_p I_{11}(p) \cos p_x \{\omega_s, \omega_d\},
\end{aligned} \tag{A.2}$$

where  $\omega_s = \cos p_x + \cos p_y$  and  $\omega_d = \cos p_x - \cos p_y$ , and the summation on  $p$  is taken over the first Brillouin zone. The functions appearing in the integrands are defined as

$$\begin{aligned}
I_1(p) &= T \sum_{\epsilon_n} G_0(p, i\epsilon_n) G_0(p, -i\epsilon_n), \\
I_2(p) &= T \sum_{\epsilon_n} G_0^2(p, i\epsilon_n) G_0^2(p, -i\epsilon_n), \\
I_3(p) &= T \sum_{\epsilon_n} G_0(p, -i\epsilon_n) G_0(p + Q, i\epsilon_n), \\
I_4(p) &= T \sum_{\epsilon_n} G_0^2(p, i\epsilon_n) G_0^2(p + Q, -i\epsilon_n), \\
I_5(p) &= T \sum_{\epsilon_n} G_0^2(p, i\epsilon_n) G_0(p, -i\epsilon_n) G_0(p + Q, -i\epsilon_n), \\
I_6(p) &= T \sum_{\epsilon_n} G_0(p, i\epsilon_n) G_0(p, -i\epsilon_n) G_0(p + Q, i\epsilon_n) G_0(p + Q, -i\epsilon_n), \\
I_7(p) &= T \sum_{\epsilon_n} G_0(p, i\epsilon_n) G_0(p + Q, i\epsilon_n), \\
I_8(p) &= T \sum_{\epsilon_n} G_0^2(p, i\epsilon_n) G_0^2(p + Q, i\epsilon_n), \\
I_9(p) &= T \sum_{\epsilon_n} G_0^2(p, i\epsilon_n) G_0(p, -i\epsilon_n) G_0(p + Q, i\epsilon_n), \\
I_{10}(p) &= T \sum_{\epsilon_n} G_0^2(p, i\epsilon_n) G_0(p + Q, i\epsilon_n) G_0(p + Q, -i\epsilon_n), \\
I_{11}(p) &= T \sum_{\epsilon_n} G_0(p, i\epsilon_n) G_0(p, -i\epsilon_n) G_0(p + Q, i\epsilon_n).
\end{aligned} \tag{A.3}$$

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